Numerical Fluid Mechanics II

Summer Semester 2021

DELIVERABLE TASK III:
Implementation of Continuous Species Transfer

Given: Monday, 07/06/2021
Deadline: 12/07/2021

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Implementation of Continuous Species Transfer (CST) in interFoam

The Navier-stokes equation for two-phase flow with volume of fluid (VOF) approach implemented in interFoam reads :

$$\nabla .u = 0 \tag{1}$$

$$\rho \left[\frac{\partial u}{\partial t} + \nabla(uu)\right] = -\nabla p + \nabla \mu \left(\nabla u + (\nabla u)^T\right) + f_b + f_{sf} \tag{2}$$

Here,

$f_b = \rho g$ and $f_s = \sigma \kappa \nabla \alpha$ are body force term and surface tension force term respectively.

- $\rho = \alpha_1 \rho_l + (1-\alpha_1)\rho_g$ mixture density
- $\mu = \alpha_1 \mu_l + (1-\alpha_1)\mu_g$ mixture viscosity

$$\alpha = \begin{cases} 1 & \text{in fluid 1} \\ 0 & \text{in fluid 2} \\ 0 < \alpha < 1 & \text{interphase} \end{cases}$$

and the VOF equation reads:

$$\frac{\partial \alpha_1}{\partial t} + \nabla\left[\alpha_1 u\right] + \nabla\left[\alpha_1(1-\alpha_1)u_r\right] = 0 \tag{3}$$

The objective of the third deliverable task is to implement continuous species transfer(CST) equation in openFoam solver interFoam. The CST equation reads as:

$$\begin{aligned} \frac{\partial C_i}{\partial t} + \nabla.(C_i U) = \nabla.(D_a \nabla C_i) - \nabla.\left(\gamma_f D_h \frac{1-\frac{1}{H}}{\alpha_1 + \frac{1-\alpha_1}{H}} C \nabla \alpha_1\right) \\ + \nabla.\left[(1-\gamma_f)(D^1 - D^2)\alpha_1 \left(\frac{1}{\alpha_1 + \frac{1-\alpha_1}{H}} - 1\right) \nabla C_i\right] \\ + \nabla.\left[(1-\gamma_f)\frac{C_i}{\alpha_1 + \frac{1-\alpha_1}{H}}\left(\frac{1}{H}\frac{D^1 - D^2}{\alpha_1 + \frac{1-\alpha_1}{H}} - \left(D^1 - \frac{D^2}{H}\right)\right)\nabla \alpha_1\right] \end{aligned} \tag{4}$$

- $D_a = D^1 \alpha_1 + D^2 \alpha_2$ arithmatic mean mixture diffusivity.
- $D_h = \frac{D^1 D^2}{\alpha_1 D^2 + (1-\alpha_1)D^1}$ harmonic mean mixture diffusivity
- $\gamma_f = |\overbrace{n_f}.\overbrace{n_\Sigma}|$; $n_\Sigma = \left(\frac{\nabla \alpha_1}{|\nabla \alpha_1|}\right)_f$; $n_f = \frac{S_f}{|S_f|}$
- Henry constant $H = C_g / C_l$.
- D^1 and D^2 diffusion coefficient of the species in the gas phase and liquid phase respectively

A group of 4 students will complete the task and submit a combined report.

Tasks

The Deliverable Task III should contain the case folder with modified solver myInterFoamCST of OpenFOAM (30p) and a written report (70p) describing the following results:

- (20p) Run simulation in a domain of height $h = 10$ cm and width 5 cm. Insert a bubble of 5 mm at 1 cm above the bottom surface with following fluid properties:

Fluid	ρ [kgm^{-3}]	μ [kgm^{-1}s^{-1}]	[ν m^{2}s^{-1}]	D cm^{2}s^{-1}	H=C_g/C_l
Water-glycerol	1205	9.45×10^{-3}	6.2241×10^{-5}	2.13×10^{-6}	33
O_2	1.122	1.824×10^{-5}	1.6257×10^{-5}	0.2085	—

  Initial $C_g = 8$ molm^{-3}
  Note: **a minimum of** 20 **grid point is necessary per bubble diameter. The CFL number should be** ≤ 0.5. A base openFoam case folder will be provided. Your task will be make necessary changes on the blockMeshDict for grid resolution, updating initial condition,PIMPLE algorith control, choice of discretization schemes and updating fvSchemes accordingly. What happens if CFL $\nleq 0.5$? do you observe any restriction on the time step size δt?

- (30p) Perform Grid Convergence Study (GCI) taking the mass transfer coefficient as variable of interest. Perform literature review on the mass transfer coefficient and how it can be calculated form numerical simulation.

- (5p) plot a contour of the concentration field at the final time.

- (15p) When a numerical simulation is bounded. Is your simulation bounded? comment and explain.

- explain your results and make your final conclusions about the Deliverable Task.

Deadline: 12th July,2021 00:00 email: md.ashfaqul.bari@fau.de